

REMARKS

Claims 1, 3-9, 11-14, 19, 21-24, 27, 29, 37, 39-45, 47-50, 55, 57-60, 63, 65 and 91-100 are pending. Claims 1, 3-7, 11-14, 19, 21, 23, 29, 37, 39-43, 47-50, 55, 57, 59, 65 and 91-100 have been amended. No new matter has added. The applicant respectfully requests reconsideration of the pending claims in light of the above amendments and the following remarks

1. Rejections under Section 112

Claims 1, 3-9, 11-14, 19, 21-14, 27, 29, 37, 39-45, 47-50, 55, 57-60, 63, 65 and 91-100 were rejected under 35 U.S.C. § 112 as allegedly being directed indefinite for failing to particularly point out and distinctly claim the subject matter of the invention. The Examiner states that the claims are indefinite because independent claims 1, 19, 37 and 55 recite the defining of “one or more destinations”, but that these and subsequent dependent claims then refer to “the defined destinations”. The applicant submits that one skilled in the art would recognize that references to “the defined destinations” refer back to the previously introduced “one or more destinations”, and that it is therefore readily apparent that these references include both the singular and the plural as dictated by their antecedent. Nevertheless, the applicant has amended claims 1, 3-7, 11-14, 19, 21, 23, 29, 37, 39-43, 47-50, 55, 57, 59, 65, and 91-100 to recite “the one or more destinations” in order to remove any possible ambiguity (and to similarly remove any possible ambiguity with respect to the various references to sources, amounts, arrangements, areas, and the like). The applicant submits that these amendments do not affect the scope of the claims. Because these amendments render the rejections under section 112 moot, the applicant requests that the rejections be withdrawn.

2. Rejections under Section 103

Claims 1, 3-9, 11-14, 19, 21-24, 27, 29, 37, 39-45, 47-50, 55, 57-60, 63, 65 and 91-100 were rejected under 35 U.S.C. § 103(a) as allegedly being unpatentable over U.S. Patent No. 6,044,212 (“Flavin”) in view of U.S. Patent No. 6,044,617 (“Schultz”) and U.S. Patent No. 6,295,514 (“Agrafiotis”). The applicant respectfully disagrees.

The present invention is based in part on the recognition of a need for tools to help scientists engaged in the discovery of new materials to design and implement libraries of candidate materials prepared by combining different chemical components, and, in particular, to visualize the vast composition spaces that result when numerous chemical components are used. To that end, the present claims recite methods and computer program products that, broadly speaking, implement graphical library design techniques in which sources (representing the chemical components) and destinations (representing substrates upon or in which materials will be prepared) are defined in a workspace of a user interface. A visual representation the destinations is displayed to the user, and the user interactively maps the chemical components to different destination locations by defining gradient distribution patterns (*e.g.*, claim 1) or systems of equations (*e.g.*, claim 19) that are used by the computer to calculate amounts of the different components that will be assigned to the different locations. The visual representation of the destinations is then modified to include a visual indication of the calculated amounts.

The Examiner recognizes that neither Flavin nor Schultz discloses the visualization techniques recited in the present claims, and points to Agrafiotis as allegedly supplying this subject matter of the claims. But, Agrafiotis is directed not to “computer design of a set of compounds”, as the Examiner suggests, but to representing the similarity or dissimilarity of a selected set of compounds. *See, e.g.*, Agrafiotis, Abstract. According to Agrafiotis, a user selects a set of compounds to be analyzed and a method for evaluating similarity/dissimilarity between the selected compounds, and the system generates a “non-linear map” that represents the set of compounds. Agrafiotis, column 2, lines 15-19. This non-linear map includes a point representing each of the selected compounds, where the “distance between any two points is representative of similarity/dissimilarity between the corresponding compounds.” *Id.*, column 2, lines 19-23. This “map” is displayed to the user, who can then interactively examine how the compounds are similar or different. *Id.*, column 2, lines 23-26.

The Examiner equates the non-linear mappings of Agrafiotis with the “mappings” of the present claims. But while Agrafiotis and the present claims may use similar words, the concepts involved are significantly different. Agrafiotis describes using non-linear mapping techniques to “visualize[e] proximity relations of objects by distances of points

in a low-dimensional Euclidean space” (*id.*, column 6, lines 63-65) – that is, to measure distances between compounds in a “similarity” space – while the present claims “map” components in the sense of assigning amounts of the components to destination cells that represent physical locations at which materials can be prepared. Nothing in Agrafiotis (or, for that matter, Flavin or Schultz) would suggest to one skilled in the art that the non-linear mapping techniques used to represent similarity/dissimilarity of compounds in Agrafiotis would be appropriate for use in assigning amounts of materials to physical library locations as contemplated by the present claims.

The Examiner also points generally to Agrafiotis’s use of a graphical user interface, and in particular to what the Examiner characterizes as “the updating or modifying ability of such an interface”. But the mere fact that Agrafiotis discloses the use of a graphical user interface to display its representation of similarity/dissimilarity of chemical compounds would not suggest the specific graphical library visualization techniques recited in the present claims. In particular, the passage the Examiner cites for the proposition of “updating or modifying” in a graphical user interface merely states that a user can modify displayed maps “by adding additional compounds to the map, removing compounds from the map, highlighting compounds on the map, etc.” Agrafiotis, column 16, lines 48-50. By contrast, the present claims recite the modification of a destination representation to include an indication of amounts of a chemical or mixture to be deposited at various cells in a destination arrangement based on a gradient or equation-based mapping. The mere fact that Agrafiotis describes its user interface as “very flexible, varied and diverse” (column 17, lines 3-4) hardly amounts to a general suggestion to use visualization techniques adapted for one purpose – to represent the *similarity or dissimilarity* of chemical compounds – for an entirely different purpose – *defining reaction parameters* as disclosed in Flavin or, for that matter, *assigning amounts* of materials to locations in a library of materials, as described in Schultz and recited in the present claims. See, e.g., *Bausch & Lomb, Inc. v. Barnes-Hind/Hydrocurve, Inc.*, 796 F.2d 443, 230 USPQ 416, 419 (Fed. Cir. 1986) (holding it is impermissible to take a single line in a prior art reference out of context); *In re Wesslau*, 353 F.2d 238, 147 USPQ 391, 393 (CCPA 1965) (“It is impermissible within the framework of section 103 to pick and choose from any one reference only so much of it as will support a given

position, to the exclusion of other parts necessary to the full appreciation of what such reference fairly suggests to one of ordinary skill in the art.”).

Moreover, even assuming Agrafiotis did disclose or suggest the visualization techniques that are not disclosed in Flavin and Schultz, there would be no motivation for one skilled in the art to combine the latter two references as the Examiner suggests. Flavin addresses the problem of optimizing chemical reactions by proposing the use of “automated synthesis methodology, product structural characterization and purity analysis, and computer-controlled design of experiments (DOE) planning and data interpretation” to accelerate the identification and optimization of chemical reactions. *Id.*, column 1, lines 62-67. “The basic concept”, according to Flavin, “is to have a machine perform the repetitive procedures involved in process development in order to increase the efficiency with which data can be collected and analyzed for a given chemical reaction.” *Id.*, column 2, lines 24-27.

To accomplish this, Flavin discloses an iterative optimization process, in which initial reactions are run, products of these reactions are automatically analyzed, and subsequent sets of experiments are iteratively and automatically generated and performed until optimum conditions are determined. *Id.*, column 4, lines 12-18. To that end, Flavin focuses on techniques that remove the user from the experimental process – in particular, automated optimization processes such as Monte Carlo and self-directed optimization techniques in which a sequence of reactions are performed in which data from one set of reactions are compared to a predetermined set of optimum criteria, and statistical techniques are used to automatically define a new set of reactions, which are then automatically performed, these results are compared to the optimum criteria and used to define still another set of reactions, and the process is repeated until no further improvement in the results is observed. *Id.*, column 5, lines 5-18; column 7, lines 17-29.

Flavin does disclose that the initial set of reactions are performed based on reagents and parameters that can be determined automatically or based on user input. *Id.*, column 5, lines 46-51. But even so, Flavin’s discussion of how these initial parameters might be defined clearly contemplates that the user would select the parameters or conditions to be investigated and the criteria by which an optimal result can be identified, and then allow the system to select particular parameter values for each experiment in the

initial set either randomly or using statistical design of experiment techniques. *See, e.g., id.*, column 4, lines 25-26 (“Optimal conditions are defined by the operator for the particular test”); column 5, lines 5-9 (use of commercial DOE programs to aid in experimental design); column 7, lines 38-41 (“the operator can define the space of parameters to be analyzed [and] run a series of random preliminary experiments”). In this context, once the parameter space and optimization conditions are defined the system takes over, automatically performing the set of reactions, analyzing the results, and defining new reactions to be performed, until the predetermined optimization conditions are obtained. *See, e.g.,* column 7, line 44-column 8, line 10.

Flavin states that its automated, iterative process is “distinctly advantageous” because it “is capable of executing significantly more tests at one time with less operator input.” *Id.*, column 4, lines 19-22. Thus, Flavin’s goal is to limit the user’s involvement in the repetitive aspects of exploring a complex experiment space and, specifically, to limit the need for user input to define the individual experiments that will be performed.

Like Flavin, Schultz discloses techniques that can be used to more efficiently study multi-variable systems. But unlike Flavin, which suggests using statistical techniques and in particular *random* selection of reaction parameters to efficiently sample a parameter space, Schultz focuses on the systematic sampling of the parameter space by preparing large numbers of materials, or performing large numbers of reactions, in parallel using uniform or systematically-varying amounts of components across a substrate array. It may be that the system disclosed in Flavin could be modified to incorporate gradient design techniques as disclosed in Schultz, but the law is clear that “[t]he mere fact that references *can* be combined or modified does not render the resultant combination obvious unless the prior art also suggests the desirability of the combination.” MPEP 2143.01 (citing *In re Mills*, 916 F.2d 680, 16 USPQ2d 1430, 1432 (Fed. Cir. 1990)). Because Flavin’s stated goal is to decrease operator involvement in the optimization process, there would be no reason for one skilled in the art modify Flavin based on Schultz and Agrafiotis in a way that would specifically require more, not less, input from the user.

The applicant therefore submits that no *prima facie* showing of obviousness has been established with respect to the present claims, and respectfully requests that the

rejections under Section 103 be withdrawn.

3. Rejections for Obviousness-Type Double Patenting


Claims 1, 3-9, 11-14, 19, 21-24, 27, 29, 37, 39-45, 7-50, 55, 57-60, 63, 65 and 91-100 were provisionally rejected under the judicially created doctrine of obviousness-type double patenting as being unpatentable over claims 89-104 of copending Application No. 09/174,856. The applicant notes that this is a provisional rejection, and will submit a terminal disclaimer at such time as the latter claims have been patented.

4. Conclusion

The applicant submits that all claims are now in condition for allowance. Please charge the fee of \$1,020.00 for a three month extension to Deposit Account 50-0496. Should any other charges be due, the Commissioner is authorized to charge the above-referenced deposit account.

Respectfully submitted,

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